

Subject: FW: CLA GW DWA Discussion
Location: 12100

Start: Wed 12/14/2016 1:00 PM
End: Wed 12/14/2016 5:00 PM
Show Time As: Tentative

Recurrence: (none)

Meeting Status: Not yet responded

Organizer: Corbin, Mark

Required Attendees: Corbin, Mark; Hetrick, James; Thurman, Nelson; Eckel, William; Cowles, James; Young, Dirk; Barrett, Michael R.; Peck, Charles; White, Katrina; Bohaty, Rochelle; Nesci, Kimberly; Villanueva, Philip; Wente, Stephen

Optional Attendees: Echeverria, Marietta (Echeverria.Marietta@epa.gov); Pease, Anita; Housenger, Jack; Keigwin, Richard; Sankula, Sujatha; Housenger, Justin; Holmes, Jean; Orrick, Greg; Spatz, Dana

-----Original Appointment-----

From: Corbin, Mark

Sent: Thursday, December 01, 2016 12:19 PM

To: Corbin, Mark; Hetrick, James; Thurman, Nelson; Eckel, William; Cowles, James; Young, Dirk; Barrett, Michael R.; Peck, Charles; White, Katrina; Bohaty, Rochelle; Nesci, Kimberly; Villanueva, Philip

Subject: CLA GW DWA Discussion

When: Wednesday, December 14, 2016 1:00 PM-5:00 PM (UTC-05:00) Eastern Time (US & Canada).

Where: 12100

This is a placeholder for the follow-up meeting with CLA with the focus here on Groundwater Modeling and DWA

Please ensure your calendar is free and plan to stay for the entire session.

Details to follow

Mark

Drinking Water Assessments- Ground Water

*EPA/CLA Meeting
December 14, 2016*



Introduction

- In our meeting on October 31, CLA discussed the problems industry has been encountering with the current drinking water assessment procedure.
 - Current procedures allow for rapid assessments using conservative assumptions with minimal effort.
 - When needed, more realistic assessments can be obtained with higher tier assessments requiring more effort.
 - A tiered assessment procedure with defined higher tiers (similar to EPA's assessment for food residues) is needed



Existing Tiered Assessment Procedures for Food and Water

Food ^a		Water ^b (Acute and Chronic)	
Acute	Chronic	Surface Water	Ground Water
Tier 1: 95 th percentile Tolerance 100% treated Default processing factor	Tier 1: point estimate Tolerance 100% treated Default processing factor	Tier A Not defined FIRST	Tier A PRZM-GW
Tier 2: 95 th percentile Field data 100% treated Study processing factor	Tier 2: point estimate Field data Maximum % treated Study processing factor	Tier B PWC (PRZM5/VVWM)	Tier B PRZM-GW: additional scenarios and degradation processes
Tier 3: 99.9 th percentile Monitoring data Maximum % treated Study processing factor	Tier 3: point estimate Monitoring data Average % treated Study processing factor	Tier C Not defined	Tier C Not defined
Tier 4: 99.9 th percentile Special studies: market basket, special processing, and PK/PD ^c studies	Tier 4 Not formally defined, but in practice similar to Tier 4 acute assessments	Tier D Not defined	Tier D Not Defined

^a Current assessment process used by EPA.

^b Existing EPA practices.

^c Special studies on pharmacokinetics (incorporate reversibility) or pharmacodynamics.

Proposed Tiered Assessment Procedures for Drinking Water

Food ^a		Water ^b (Acute and Chronic)	
Acute	Chronic	Surface Water	Ground Water
Tier 1: 95 th percentile Tolerance 100% treated Default processing factor	Tier 1: point estimate Tolerance 100% treated Default processing factor	Tier A Not defined FIRST	Tier A PRZM-GW
Tier 2: 95 th percentile Field data 100% treated Study processing factor	Tier 2: point estimate Field data Maximum % treated Study processing factor	Tier B PWC (PRZM5/VVWM)	Tier B PRZM-GW with additional scenarios and degradation processes
Tier 3: 99.9 th percentile Monitoring data Maximum % treated Study processing factor	Tier 3: point estimate Monitoring data Average % treated Study processing factor	Tier C: PWC (PRZM5/VVWM) with refinements, spatial assessments	Tier C: PRZM-GW: additional processes/lab studies/field studies; spatial assessments
Tier 4: 99.9 th percentile Special studies: market basket, special processing, and PK/PD ^c studies	Tier 4 Not formally defined, but in practice similar to Tier 4 acute assessments	Tier D Monitoring data interpreted by refined modeling	Tier D Monitoring data interpreted by refined modeling

^a Current assessment process used by EPA.

^b Combination of existing EPA practices (Tiers A and B) and CropLife America proposals (Tiers C and D)

^c Special studies on pharmacokinetics (incorporate reversibility) or pharmacodynamics.

Introduction

- Today's discussion will focus on drinking water from ground water sources.
 - An introductory presentation will discuss the major areas of concern.
 - A presentation on development of additional scenarios
 - Case studies will be used to illustrate the process for three compounds.
- While the case studies show potential approaches for some compounds, CLA wants to open a dialogue with EPA on approaches that provide more predictive estimates while meeting EPA concerns for adequate protection.



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History

- Drinking water assessments were originally performed with SCI-GROW
 - A regression of compound properties with results of prospective ground water studies.
 - For all but a few low Koc compounds, the drinking water assessments were controlled by residues in surface water.



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History

- Since 2012 PRZM-GW has been used for drinking water assessments.
 - Generally much higher predictions than SCI-GROW
 - ❖ Some relief with the introduction of hydrolysis
 - Ground water controls the drinking water assessment much more frequently than when SCI-GROW was used
 - Persistent and relatively immobile compounds also trigger ground water concerns
 - Industry's concerns are not with the model but with the conservative parameterization
 - ❖ Appropriate for initial simulations
 - ❖ Need to work with EPA to find way to use higher tier data when available to conduct more predictive simulations



Potential Approaches to Refined Assessments

- Definition of additional crop-specific and geographically specific scenarios
 - EFED has included this as a potential option for higher tier assessments
 - Especially helpful when the scenario is not relevant to the use of the specific compound
 - ❖ Otherwise this area would be subject to label mitigations
- Approaches that achieve more predictive simulations are also needed



Potential Approaches to Refined Assessments

- Degradation
 - Degradation as a function of depth
 - ❖ Includes soils, subsoils, and ground water
 - Use of DFOP kinetics
- Sorption processes
 - Freundlich
 - Time-dependent sorption
- Such refinements can easily be implemented in existing EPA models.



Degradation as a Function of Depth

- This is a topic where CLA is not aware of a definitive answer on how degradation rates change with depth.
 - The correct description may be compound-specific.
- We commend EPA for including it as a topic on the next EMPPM in the spring.



Degradation as a Function of Depth

- Degradation has long been assumed to decrease with depth
 - Reduced soil microbes
- In practice this has been difficult to determine under field conditions except for mobile compounds
 - Field studies conducted with aldicarb, isoxaflutole, thiodicarb, and ethoprop have shown little or no decrease in degradation with depth in the upper 3-5 meters of soil
 - ❖ Exceptions include very coarse sands (but not fine sands)



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Degradation as a Function of Depth

- This effect is difficult to determine in laboratory studies
 - Perhaps because subsoil conditions are hard to maintain in the laboratory, resulting in stresses to soil microbes
 - A field study conducted with aldicarb showed no change with depth, while laboratory degradation studies with soils from the same location did show slower degradation rates in subsoils.



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PRZM-GW1.07 Adjustment Factors for Aerobic Degradation

Soil Depth (cm)	Adjustment Factor
0-10	1
10-20	0.94
20-40	0.78
40-60	0.55
60-80	0.33
80-100	0.11
Below 100	0

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Degradation as a Function of Depth

- The current parameterization of degradation as a function of depth is conservative but probably appropriate as a starting point
- Industry would like to work with EPA to develop an approach to more realistic approaches based on compound specific information, perhaps including
 - Use of field data when available for mobile compounds.
 - Design of studies to obtain information on degradation with depth for less mobile compounds such as long term hydrolysis studies.
 - Options for compounds stable to hydrolysis

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Degradation in Ground Water

- We appreciate the option in PRZM-GW to calculate the decline in the peak as a function of distance away from the field and would hope that EPA will retain this option.

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Use of DFOP Kinetics

- For mobile compounds that do not follow single first order kinetics, representing the measured kinetics can provide a more realistic assessment. DFOP (double first order in parallel) kinetics can be implemented in PRZM-GW
 - For simulations using linear adsorption, no model modifications are needed to implement DFOP kinetics.
 - Minor modifications are needed to implement DFOP simulations with Freundlich sorption (but versions of PRZM exist which implement these modifications).

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Sorption

- In the discussions around Freundlich and aged (time-dependent) sorption, there have been discussions on whether degradation occurs in the liquid phase or in both the liquid and solid phases.
- The following slides present some work done in response to this topic (presented in a poster at SETAC on November 8, 2016).
 - Jones, R. L., R. Sur, E. Henry, B. Jene, and W. Chen. 2016. Importance of Time-Dependent Sorption in Ground Water Modeling in Regulatory Assessments. Poster TP172 at the 7th SETAC World Congress, Orlando, 6-10, 2016



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Degradation Location-Introduction

- The degradation of pesticides is a complex process so laboratory studies measure overall degradation rates.
 - Degradation may be occurring in the liquid or solid phase compartments or at the liquid-solid interface
- Regulatory models are usually parameterized with this overall rate being the degradation rate in both the liquid and solid phases.
- Two exercises were done to help explore whether degradation was occurring only in the liquid phase



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Effect of Organic Matter

- Premise:
 - If degradation occurred only in the liquid phase and is not a strong function of soil organic matter, then increasing organic matter would result in slower degradation because less compound would be present in the liquid phase.
- Data set:
 - 7 active ingredients
 - 12 soils,
 - 34 individual values of DT50

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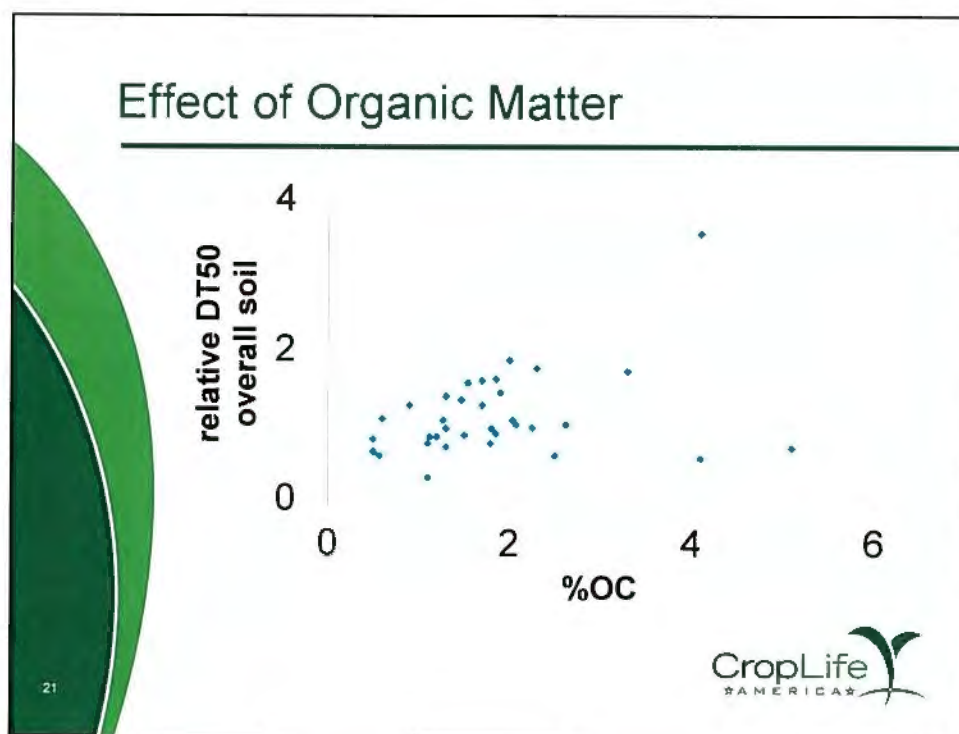


Effect of Organic Matter

- For each of the 35 DT50 values, a relative DT50 value was calculated.
 - Each relative DT50 represents the ratio of the individual DT50 to the geometric mean of all of the individual DT50s available for the specific active ingredient

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Effect of Organic Matter

- There is no trend of increasing of DT50 ratios with increasing organic carbon.
- Therefore this exercise does not support the conclusion that degradation only occurs in the liquid phase.

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Variability of Degradation Rates

- Premise:
 - If degradation occurred only in the liquid phase and was not a strong function of soil organic matter, the variation in degradation rates in different soils for the same active ingredient would be less when degradation rates are expressed as liquid phase degradation rates than when expressed as overall degradation rates.
- Data set:
 - 6 active ingredients
 - 16 soils
 - 58 individual values of DT50



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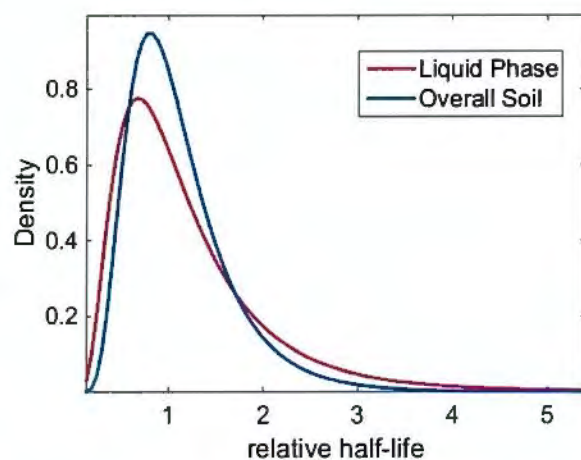
Variability of Degradation Rates

- For each of the 58 DT50 values, a relative DT50 value was calculated.
 - Each relative DT50 represents the ratio of the individual DT50 to the geometric mean of all of the individual DT50s available for the specific active ingredient



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Variability of Degradation Rates



Variability of Degradation Rates

- The 90% confidence interval of the natural logarithm of the geometric mean was 0.90-1.11 for the overall degradation rates and 0.87-1.15 for the liquid phase degradation rates
- The variability of the degradation rates expressed as an overall degradation rate is slightly less than when expressed as a liquid degradation rate.
- Therefore this exercise does not support the conclusion that degradation only occurs in the liquid phase.

Conclusion-Degradation Location

- There is no evidence from analyses conducted in these two exercises that degradation of active substances of crop protection products and their metabolites only occurs in the liquid phase of the soil.



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Freundlich Sorption

- For many compounds the Koc increases with decreasing concentrations.
- Freundlich sorption has been used for many years to describe sorption data generated for registration
- Freundlich sorption has been used for many years in pesticide modeling around the world
 - Also an option available in PWC, but not activated



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Introduction: Time-Dependent Sorption

- Scientists have recognized for over 40 years that sorption of many active ingredients of crop protection products and their metabolites to soil increases with time.
- This process is typically referred to as time-dependent sorption (TDS), aged sorption, kinetic sorption, or non-equilibrium sorption.
- This increase in sorption slows the downward movement of compounds through the soil profile.

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Introduction: Time-Dependent Sorption

- Introduced into PEARL in 2000 as an option in FOCUS modeling for European registrations
 - Later introduced into the other models used in FOCUS modeling (PELMO, MACRO, and FOCUS PRZM)
- Also an option available in PWC, but not activated

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Modeling of TDS

- Currently TDS is modeled in a pragmatic way considering a liquid phase and two solid phase compartments, one in equilibrium with the liquid phase and the other where sorption is kinetically controlled.
- The solid phase compartment in equilibrium with the liquid phase and the liquid phase both have equal degradation rates.
- Sorption and desorption between the kinetically controlled solid phase compartment and the liquid phase is described by mono-exponential kinetics.



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Modeling of TDS

- Usually bioavailability is assumed to be very low in the kinetically controlled solid phase compartment so no degradation occurs.
- Five variables have been traditionally used to model this process, which are determined by regression of results from a specifically designed aged sorption laboratory experiment



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Modeling of TDS

- M_{ini} initial mass
- $DegT50_{EQ}$ degradation in liquid and soil equilibrium phases
- $K_{OM,EO}$ sorption between liquid and soil equilibrium phases
- f_{NE} ratio between the non-equilibrium and equilibrium Freundlich coefficients
- k_{des} desorption rate coefficient

- The number of variables can be reduced to four by setting $K_{OM,EO}$ to the value measured after 24 hours



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Laboratory TDS Studies

- EPA has expressed concern about the quality of laboratory studies used to derive time-dependent sorption parameters
 - Guidance exists, sponsored by the UK CRD, on the conduct of aged sorption studies, as well as the application of the results of these studies to development of modeling parameters for time-dependent sorption.



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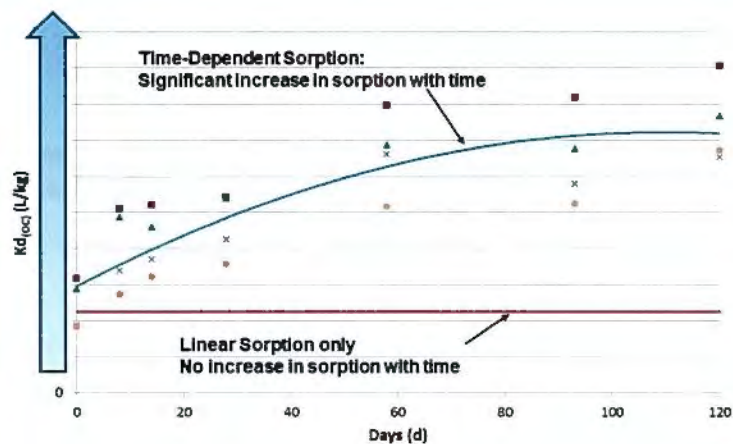
Example

- Insecticide applied to sucking pests on a field typically planted with potatoes for two years rotated with corn for one year
- Monitored for 15 years
- Highly vulnerable aquifer on Long Island, NY. Soil is Riverhead sandy loam
- Depth to ground water: 7.1 m; Well screen: 6.1-9.1 m below the soil surface

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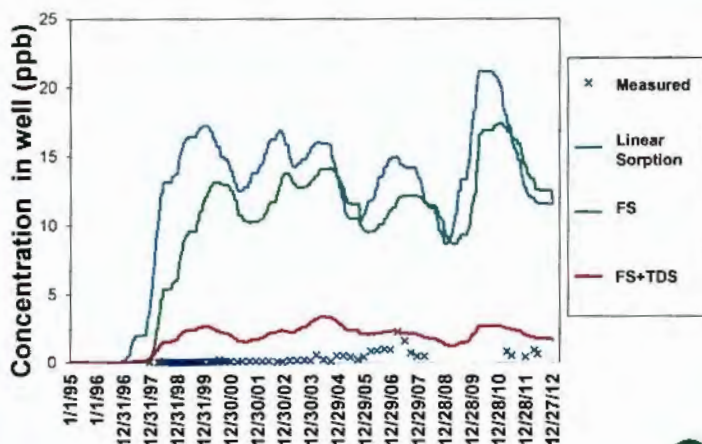
Results of Time-Dependent Sorption Study



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Comparison of Modeling and Monitoring Results



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Example Conclusions

- The use of Freundlich and time-dependent sorption brings the predicted values much closer to the monitoring data and more reflective of actual exposure
 - Further improvement occurs if the degradation rate measured in field studies is used rather than the rate from laboratory studies

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Concluding Remarks

- Today's discussion will focus on drinking water from ground water sources.
 - A presentation on development of additional scenarios
 - Three presentations showing case studies
 - A few summary slides with conclusions
- We hope that today's discussions on ground water will identify some mutually acceptable options for providing more realistic estimates of drinking water concentrations for use in refined human health risk assessments

